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NBS Technical Note 1244

Thermodynamic Properties of Halides, Hydrides, and Deuterides of Cobalt, Iron, and Nickel I. Literature Citations

Cynthia R. Jackson and Malcolm W. Chase

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Chemical Thermodynamics Data Centers
Chemical Thermodynamics Division
Center for Chemical Physics
National Measurement Laboratory
National Bureau of Standards
Gaithersburg, MD 20899

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THERMODYNAMIC PROPERTIES OF HALIDES, HYDRIDES, AND DEUTERIDES OF COBALT, IRON, AND NICKEL
I. Literature Citations

Table of Contents

ABSTRACT

A bibliographic collection is provided on data which are necessary for the calculation of the thermochemical properties of the gaseous metal halides, hydrides (deuterides) and their positive and negative ions (MX, MX^+ and MX^-), where M = Co, Fe, and Ni and X = Br, Cl, F, H(D), and I. This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties of these substances for the JANAF Thermochemical Tables.

The collection contains references which have been published through the end of 1986 with some 1987 references. Fifteen bibliographies are given, one for each species. In all bibliographies, the references are listed chronologically; alphabetically by first author within each year. The names of the species are given according to the Chemical Abstracts system of nomenclature (as of the Tenth Collective Index) when possible. The Chemical Abstracts Registry Numbers, if assigned, are also given for each of the species. A brief summary of the type of available information is given.

Keywords: bibliography, electron affinity, electronic energy levels, equilibrium data, formation properties, ionization potential, molecular structure, review articles, thermochemistry, thermodynamic properties, transition metal halides and hydrides, vibrational frequencies

INTRODUCTION

This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties of chemical species for the JANAF Thermochemical Tables. In this particular article, thermochemical tables for the gaseous iron, cobalt and nickel halides, hydrides (deuterides) and their positive and negative ions (MX, MX^+, MX^-) are being prepared. The iron species are also being studied for use in the CODATA Task Group on Chemical Thermodynamics Tables. The preparation of these thermochemical tables has been divided into a series of sequential sections, each section containing documentation. This permits the technical community not only to have access to all the available pertinent references early in the investigation but also to view the progress in the critical evaluation of the thermodynamic properties for the JANAF Thermochemical Tables. It is hoped that this will stimulate interested scientists to comment on the documentation so that we can make it as complete as possible. The goal is to construct a complete bibliographic resource, upon which future studies can be built, and to eliminate the need for another search of the past literature on these species. In the future, one only should have to be concerned with current updates to this survey. A possible limitation in this coverage is in the appearance of pertinent data in journals not accessed by the abstracting services.

In general, the first two steps involve the construction of the bibliographies, followed by a set of data summaries (i.e., summaries of the reported data in tabular and graphical format). Subsequently, there will be published preliminary thermal functions, preliminary formation properties, and then the final thermochemical tables. The latter normally would be a fine-adjustment of the preliminary values. This fine-adjustment would result from the examination of data consistency as viewed from a larger group of species, i.e. a mathematical solution of a thermochemical network or consideration of trends in the periodic table. From a network solution, there is obtained a statistical assessment of the overall uncertainties in the formation properties and a better understanding of the interconsistency of all data used in the network. In the species studied here, however, the data are not strongly linked via chemical reactions to other species. Thus, a network solution may not be necessary. However, a comparison of the results of this study with the results for other transition metal species would be beneficial in confirming possible trends and identifying possible discrepancies.

NOMENCLATURE

The species of interest in this bibliographic collection are given below with their names and registry numbers, as obtained from Chemical Abstracts On-Line (Registry File) in October 1987. Only 31 of the potentially relevant 54 species have been assigned registry numbers. The remaining 23 species, which are not listed in the following table, are named in analogy with those given. Historically, these species have often been called monohalides, monohydrides, and monodeuterides, but these designations are not used. In addition, names such as "chloronickel ion" have been used in the past but are no longer used by Chemical Abstracts. Although our intent was to cover the positive and negative ions of the above mentioned eighteen neutral species, not all of these species have been listed in the Chemical Abstracts Registry Number system, and thus are not listed here. Interestingly, there is no data reported in Chemical Abstracts for NiI(g), but there is information for the positive ion. On the other hand, data are given in the literature for FeI^+, but no access to this species is given in Chemical Abstracts through the Formula Index.

formula	name	registry number
CoBr	Cobalt Bromide	22584-72-1
CoCl	Cobalt Chloride	34240-80-7
CoCl+	Chlorocobalt(1+)	52082-14-1
CoD+	Hydro-d-cobalt(1+)	87136-05-8
CoD	Cobalt Hydride (CoD)	76622-37-2**
CoD	Cobalt Hydride (CoD)	40418-24-4**
CoD	Cobalt Deuteride	37362-92-8**
CoF	Cobalt Fluoride	67321-83-9
CoF+	Fluorocobalt(1+)	21773-33-1
CoH	Cobalt Hydride	14994-20-8
CoH+	Hydrocobalt(1+)	12378-09-5
CoH-	Hydrocobaltate(1-)	65899-90-7
CoI	Cobalt Iodide	101015-09-2
FeBr	Iron Bromide	12514-32-8
FeBr+	Bromoiron(1+)	90143-36-5
FeCl	Iron Chloride	27846-09-9
FeD	Iron Deuteride	40418-23-3
FeF	Iron Fluoride	41428-55-1
FeH	Iron Hydride	15600-68-7
FeH+	Hydroiron(1+)	71899-96-2
FeH-	Hydroferrate(1-)	64899-88-3
FeI	Iron Iodide	33019-21-5
NiBr	Nickel Bromide	71939-11-2
NiCl	Nickel Chloride	13931-83-4
NiCl+	Chloronickel(1+)	52082-15-2
NiD	Nickel Deuteride	14989-21-0
NiD+	Hydro-d-nickel(1+)	75181-24-7

NiF	Nickel Fluoride	13783-64-7
NiF+	Fluoronickel(1+)	26024-87-3
NiH	Nickel Hydride	14332-32-2
NiH+	Hydronickel(1+)	75181-25-8
NiH-	Hydronickelate(1-)	64899-92-9
NiI+	Iodonickel(1+)	53290-74-7

** NOTE: There are three registry numbers assigned to CoD.

LITERATURE COVERAGE

All references, which appear to have some data pertinent to the thermochemical calculations, have been collected into fifteen bibliographies, one for each of the halides and hydrides (deuterides) of cobalt, iron and nickel. The references for the deuterides are contained in the hydride bibliographies. These references were taken primarily from a search of Chemical Abstracts, from the First Collective Index, which includes 1907-1916, to the 11th Collective Index, which includes 1982-1986. However, we have included some 1987 publications in the bibliographies. In addition, scanning of the retrieved articles, manual scanning of selected resources, using personal contacts, searching the Chemical Thermodynamics Data Centers abstract files, and searching the Ion Kinetics and Energetics Data Center data base have yielded additional publications. It is hoped that the collection is complete through 1986 within the following constraints:

1. Articles referring to aqueous solutions involving MX^+ and MX^- usually are not included. We are interested only in the gaseous MX, MX^+ and MX^- species.

2. Articles referring to estimated thermochemical values for MX(cr) are not included.

3. Articles published in astrophysical journals often are not included since they usually are not presenting new spectral information. More often, existing spectral data are given.

4. Analytical chemistry articles which deal with the interferences of MX(g) electronic bands with other bands typically are not included. These articles normally do not give definitive values for the electronic bands nor do they present data relevant to this particular thermodynamic study.

5. Articles using existing thermochemical values for the hydrides (deuterides) and halides in calculations are not included, unless the article includes a discussion of problems in the calculated results.

6. At this time, only those critical reviews which deal exclusively with halides and hydrides (deuterides) are included. The more general critical reviews (i.e. JANAF Thermochemical Tables) will be included in the next publication of this series.

The inclusion of an article in this collection does not necessarily imply that it will be of high importance in the final selection of data. Since there is not an overabundance of data, we have been unselective in our choice of entries in these bibliographies, and have extracted some articles which are tangential to our work with the hope that some useful information may be hidden in them. The initial examination of the literature suggests that sufficient reliable information is not available to generate sound thermochemical tables for some halides and hydrides (deuterides). Many will be estimated tables.

In generating these bibliographic files, the intent is to add information progressively as the evaluation procedure progresses. Thus, starting with this article, the prime effort is to list authors and the journal citation. As the literature searching proceeds and as articles are obtained, additional information will be added (e.g., article title, Chemical Abstracts reference). Thus, some citations may be incomplete at this time. Eventually, the majority of the bibliographic citations will (should) contain:

authors
title of article
journal citation
abstract citation (Chemical Abstracts, Physics Abstracts, etc.)
short annotation as to information in the article

At this time for these metal halides and hydrides (deuterides), we have collected the majority of the available data, with no statement as to its reliability or usefulness.

DATA SUMMARIES

The next publication in this series will contain sets of tabular information which will summarize the relevant data, as presented in the original publication. These summaries will help direct attention to the data actually available for use in generating thermochemical tables. In the case of these halides and hydrides (deuterides), data summaries will be presented for the following information:

dissociation energy
electronic energy levels and configurations
vibration-rotation constants
ionization potential
electron affinity

The same information will be summarized for the positive and negative ions. In all cases, experimental and theoretical data are included.

The following table summarizes briefly the nature and quantity of data available for the halides and hydrides (deuterides).

SUBJECT COVERAGE IN REFERENCES ON COBALT, IRON, AND NICKEL SPECIES

	CoBr	CoCl	CoD	CoF	CoH	CoI
total references	7	13	8	4	29	1
electronic energy information						
electronic energy levels	6	9	4	-	11	-
vibrational analysis	4	7	2	-	9	-
rotational analysis	-	-	3	-	-	-
dissociation energy	-	1	-	1	12	1
ionization potential	-	-	1	1	2	-
electron affinity	-	-	1	-	-	-

	FeBr	FeCl	FeD	FeF	FeH	FeI
total references	6	21	7	17	44	3
electronic energy information						
electronic energy levels	4	11	3	3	15	-
vibrational analysis	4	8	1	-	7	-
rotational analysis	-	1	1	1	-	-
dissociation energy	-	6	1	5	20	1
ionization potential	-	-	1	-	3	3
electron affinity	-	-	1	-	1	-

	NiBr	NiCl	NiD	NiF	NiH	NiI
total references	15	27	10	15	48	1
electronic energy information						
electronic energy levels	10	14	3	7	19	-
vibrational analysis	9	14	2	3	14	-
rotational analysis	-	1	2	2	3	-
dissociation energy	1	7	1	3	17	3
ionization potential	-	1	1	-	3	-
electron affinity	1	1	1	-	-	-

Since any one article may contain information pertaining to more than one category listed on the previous page, the sum within any column will not necessarily equal the total. In addition, some articles do not report any data, but instead discuss the interpretation of previously reported data.

ACKNOWLEDGEMENT

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37MES Mesnage, P., "Molecular emission spectra of some metallic salts", Compt. Rend., 204, 1929-1931 (1937), CA31:6108(8), emission spectra, electronic energy levels

39MES Mesnage, P., "Researches on high-frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), vibrational analysis, emission spectra, electronic energy levels

52KRI Krishnamurty, V.G., "Structure of the band spectra of the halides of Co and Ni", Dissertation, Univ. Andhra, Doctoral Thesis (1952), emission spectra, electronic energy levels

62RAO/RAO Rao, S.V.K., Rao, P.T., "The spectrum of CoBr in the visible (4300-4700 A.)", Indian J. Phys., 36, 609-612 (1962), CA59:3442b, emission spectra, electronic energy levels, vibrational analysis

68RAO/RAO Rao, N. V. K., Rao, P. T., "New band systems of CoBr in the photographic infrared", Curr. Sci., 37(21), 608-609 (1968), CA70(12):52722b, emission spectra, vibrational analysis, electronic energy levels

72RAO/RED Rao, N. V. K., Reddy, Y. P., Rao, P. T., "Emission spectrum of CoBr in the visible region", Indian J. Pure Appl. Phys., 10(5), 389-391 (1972), CA77(22):145832x, emission spectrum, vibrational analysis, electronic energy levels

86KHA/GER Kharitonov, Yu. Ya., Gerzha, T. V., Averbukh, B. S., Kuznetsov, S. L., "Thermodynamic properties of gaseous di-and monohalides of iron, cobalt and nickel", Zh. Neorg. Khim., 31(7), 1679-1682 (1986), CA105(14):121784d, Eng. transl., Russ. J. Inorg. Chem., 31(7), 961-963 (1986), thermodynamic properties

12POL Pollok, J.H., "Vacuum tube spectra of some metals and metallic chlorides. II. Lead, iron, manganese, nickel, cobalt, chromium, barium, calcium, strontium, magnesium, potassium, sodium and lithium", J. Chem. Soc., 102(Pt.2), 710-711 (1912), CA7:1132(8), spectra, electronic energy levels, see also Sci. Proc. Roy Dubl. Soc., 13, 253-268 (1912)

35MES Mesnage, P., "Molecular emission spectra of some metallic salts", Compt. Rend., 201, 389-391 (1935), CA29:6503(2), emission spectra, electronic energy levels

37MOR More, K.R., "Band spectra of NiCl and CoCl", Phys. Rev., 51, 1019 (1937), CA32:5294(4), emission spectra, electronic energy levels

38MIE Miescher, E., "Molecular spectra of halogens of the ion group, particularly FeCl", Helv. Phys. Acta, 11, 463-468 (1938), emission spectra

38MOR More, K.R., "Spectra of the monochlorides of nickel, cobalt and iron", Phys. Rev., 54, 122-125 (1938), CA32:7342(9), vibrational analysis, emission spectra, electronic energy levels

39MES Mesnage, P., "Researches on high-frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), emission spectra, vibrational analysis, electronic energy levels

51KRI Krishnamurty, V.G., "$^5\Pi$-$^5\Sigma$ electronic transition in cobalt chloride", Curr. Sci. (India), 20, 323 (1951), CA46:4908a, emission spectra, vibrational analysis, electronic energy levels, see also CA47:1487c

52KRI Krishnamurty, V.G., "$^5\Pi$-$^5\Sigma$ electronic transition in cobalt chloride", Indian J. Phys., 26, 177-185 (1952), CA47:1487c, emission spectra, vibrational analysis, electronic energy levels, see also CA46:4908a

61RAO/RAO Rao, S.V.K., Rao, P.T., "The spectrum of CoCl in the photographic infrared and in the visible", Indian J. Phys., 35, 556-561 (1961), CA57:283c, emission spectra, vibrational analysis, electronic energy levels

71KUL/DAD Kulkarni, M. P., Dadape, V. V., "Sublimation pressure of cobalt dichloride and the study of the reaction cobalt(c) + cobalt dichloride (g)=cobalt monochloride (g) at high temperatures", High Temp. Sci., 3(4), 277-282 (1971), CA75(18):113319c, enthalpy of formation

72BOR/BUL Borisov, Yu.A., Bulgakov, N.N., "Semiempirical method for calculating bond energies", Zh. Strukt. Khim., 13(1), 103-110 (1972), CA76(20):117733b, Eng. transl., J. Struct. Chem., 13, 89-95 (1972), dissociation energy

83GRE/MCD Green, D.W., McDermott, D.P., Bergman, A., "Infrared spectra of the matrix-isolated chlorides of iron, cobalt, and nickel", J. Mol. Spectrosc., 98(1), 111-124 (1983), CA98(20):169624r, matrix isolation study, vibrational analysis

84RED/NAR Reddy, C. V., Narayana, A. L., Rao, P. T., "The emission spectrum of cobalt chloride (CoCl) in the visible region", Optica Pura Aplicada, 17(3), 289-296 (1984), CA102(22):194359s, emission spectra, vibrational analysis, electronic energy levels

84RED/NAR2 Reddy, C. V., Narayana, A. L., Rao, P. T., "Spectrum of cobalt monochloride (CoCl) in the visible region λλ 5350-5900 P", Indian J. Pure Appl. Phys., 22(9), 550-552 (1984), CA101(24):218921b, emission spectra, vibrational analysis, electronic energy levels

66KAN/BES Kana'an, A.S., Besenbruch, G., Margrave, J.L., "Knudsen and Langmuir measurements of the sublimation pressure of CoF_2", J. Inorg. Nucl. Chem., 28, 1035-1037 (1966), CA64:18442h, dissociation energy

68SAA/MCD Saalfeld, F. E., McDowell, M. V., Hagen, A. P., MacDiarmid, A. G., "Mass spectrum of trifluorosilyltetracarbonylcobalt", Inorg. Chem., 7(8), 1665-1667 (1968), CA69(16):62803x, appearance potential

70SAA Saalfeld, F.E., "Energetics of electron impact reactions", Rep. NRL (Nav. Res. Lab.) Progr., Feb. 1-7 (1970), CA72(24):126367e, formation

78DEV/VAN DeVore, T. C., Van Zee, R. J., Weltner, W., Jr., "An investigation of the first row transition - metal fluoride molecules using ESR spectroscopy", Proc. - Electrochem. Soc., Proc. Symp. High Temp. Met. Halide Chem., 1977, 78-1, 187-198 (1978), CA89(14):120290d, no data

31JOH/JOH Johnson, L.W., Johnson, R.C., "Band spectrum of YtO-ScO and LaO systems", Proc. Roy. Soc. London, 133, 207 (1931), CA25:5843, emission spectra

36HEI Heimer, A., "Band spectra of NiH and CoH", Naturwissenschaften, 24, 413 (1936), CA31:33(9), emission spectra

37HEI Heimer, A., "The band spectrum of cobalt hydride", Z. Physik, 104, 448-457 (1937), CA31:3383(8), emission spectra

37HEI2 Heimer, A., Thesis, Stockholm (1937), spectra

46GUG Guggenheimer, K.M., "New regularities in vibrational spectra", Proc. Phys. Soc. (London), 58, 456-468 (1946), CA40:6991(5), emission spectra

59VAR/MIT Varshni, Y.P., Mitra, S.S., Shukla, R.C., "Spectroscopic constants of molecules. VII. Relation between force constant and equilibrium internuclear distance for hydride diatoms", Indian J. Phys., 33, 473-482 (1959), CA54:10496a, bond length

63KLY/NEU Klynning, L., Neuhaus, H., "The band spectrum of CoD", Z. Naturforsch., 18a, 1142 (1963), CA60:4970e, emission spectra

65CAR/CAR Carbo, R., de Carbo, C.A., Molina, J., "Calculation of the energy of the ground state of diatomic molecules by an L.C.A.O.-S.C.F. method", Afinidad, 22(240), 403-405 (1965), CA64:18677e, electronic energy levels

66POL Politzer, P., "Bond lengths and atomic orbital radii in the diatomic hydrides", J. Phys. Chem., 70(12), 4041-4044 (1966), CA66(6):22408d, bond length

73KLY/KRO Klynning, L., Kronekvist, M., "New subsystem in the band spectrum of cobalt monodeuteride", Phys. Scr., 7(1-2), 72-74 (1973), CA78(24):153428f, rotational analysis, electronic energy levels

73SMI Smith, R. E., "Diatomic hydride and deuteride spectra of the second row transition metals", Proc. Roy. Soc. London, Ser. A, 332(1588), 113-127 (1973), CA78(12):77638g, spectra

76JEN/JON Jensen, D.E., Jones, G.A., "Aspects of the flame chemistry of cobalt", J. Chem. Soc., Faraday Trans. 1, 72(11), 2618-2630 (1976), CA86(12):79337x, enthalpy of formation

77MID Middleton, R., "A survey of negative ions from a cesium sputter source", Nucl. Instrum. Methods, 144(3), 373-399 (1977), CA87(24):190803f, formation

77MIN/FOR Mingos, D. M. P., Forsyth, M. I., "Molecular-orbital calculations on transition-metal cluster compounds containing six metal atoms", J. Chem. Soc., Dalton Trans., (6), 610-616 (1977), CA87(4):29280y, structure

80KHA/KRA Kharitonov, Yu. Ya., Kravtsova, G. V., "Empirical dependences between force constants and bond length for iron, cobalt, and nickel hydrides", Zh. Neorg. Khim., 25(11), 3053-3058 (1980), CA94(12):92726h, Eng. transl., Russ. J. Inorg. Chem., 25, 1676-1679 (1980), force constant, bond length

81ARM/BEA Armentrout, P. B., Beauchamp, J. L., "Ion beam studies of the reactions of atomic cobalt ions with alkanes: determination of metal-hydrogen and metal-carbon bond energies and an examination of the mechanism by which transition metals cleave carbon-carbon bonds", J. Am. Chem. Soc., 103(4), 784-791 (1981), CA94(15):120457s, dissociation energy

81ARM/HAL Armentrout, P.B., Halle, L.F., Beauchamp, J.L., "Periodic trends in transition metal-hydrogen, metal-carbon, and metal-oxygen bond dissociation energies. Correlation with reactivity and electronic structure", J. Am. Chem. Soc., 103(21), 6501-6502 (1981), CA95(18):156742r, dissociation energy, ionization potential

81DAS Das, G., "A pseudopotential study of the iron-series transition metal hydrides", J. Chem. Phys., 74(10), 5766-5774 (1981), CA95(2):13166v, dissociation energy

81KAN/MOO Kant, A., Moon, K.A., "Mass spectrometric determination of the dissociation energies of gaseous aluminum hydride, gallium hydride, indium hydride, scandium hydride, and cobalt hydride and estimation of the maximum dissociation energies of thallium hydride, chromium hydride, manganese hydride, and iron hydride", High Temp. Sci., 14(1), 23-31 (1981), CA95(12):103738n, dissociation energy

81KHA/KRA Kharitonov, Yu. Ya., Kravtsova, G. V., "Thermodynamic functions of diatomic hydrides of Group VIII metals", Zh. Neorg. Khim., 26(5), 1198-1201 (1981), CA95(4):31394x, Eng. transl., Russ. J. Inorg. Chem., 26, 645-647 (1981), thermodynamic properties

JANAF THERMOCHEMICAL TABLES - COBALT BIBLIOGRAPHIES
COBALT HYDRIDE (CoH, CoH^+, CoH^-)

81KLY/KRO Klynning, L., Kronekvist, M., "Rotational analysis of the 4547 P and 4548 P bands of cobalt hydride (CoH)", Phys. Scr., 24(1,Pt.1), 21-22 (1981), CA95(14):123449x, rotational analysis

81NIC Nicholls, R. W., "Franck-Condon factor formulas for astrophysical and other molecules", Astrophys. J., Suppl. Ser., 47(3), 279-290 (1981), CA96(8):60604s, Franck-Condon factors

83CAR/SAL Carlin, T.J., Sallans, L., Casssady, C.J., Jacobson, D.B., Freiser, B.S., "Gas-phase reactions of Group VIII metal hydride ions (FeD^+, CoD^+, and NiD^+) with hydrocarbons", J. Am. Chem. Soc., 105(20), 6320-6321 (1983), CA99(17):140141r, ionization potential

83RAJ/RAT Rajulu, A.V., Ratnam, S.R., Reddy, R.R., "Electronegativities in the calculation of diatomic molecular parameters (hydrides of some transition elements)", J. Quant. Spectrosc. Radiat. Transfer, 29(1), 85-88 (1983), CA98(8):62295g, electron affinities

84MAN/HAL Mandich, M. L., Halle, L. F., Beauchamp, J. L., "Determination of the metal-hydrogen and metal-methyl bond dissociation energies of the second-row, Group 8 transition metal cations", J. Am. Chem. Soc., 106(16), 4403-4411 (1984), CA101(9):72937n, dissociation energies

84SAU/TAT Sauval, A. J., Tatum, J. B., "A set of partition functions and equilibrium constants for 300 diatomic molecules of astrophysical interest", Astrophys. J., Suppl. Ser., 56(2), 193-209 (1984), CA101(22):200866c, thermodynamic properties

85BOR/TYU Borodyuk, N. R., Tyulin, V. I., "Calculation of lower limit for the equilibrium internuclear distances in excited electronic states of diatomic molecules", Vestn. Mosk. Univ., Ser. 2: Khim., 26(6), 546-551 (1985), CA104(16):138351n, bond length

85SAL/LAN Sallans, L., Lane, K.R., Squires, R.R., Freiser, B.S., "Generation and reaction of atomic metal anions in the gas phase. Determination of the heterolytic and homolytic bond energies for the vanadium, chromium, iron, cobalt, and molybdenum hydrides VH, CrH, FeH, CoH, and MoH", J. Am. Chem. Soc., 107(15), 4379-4385 (1985), CA103(6):42997f, dissociation energy

86CHI/LAN Chiong, D.P., Langhoff, S.R., Bauschlicher, C.W., Jr., Walch, S.P., Partridge, H., "Theoretical dipole moments for the first-row transition metal hydrides", J. Chem. Phys., 85(5), 2850-2860 (1986), CA105(18):163141x, dipole moment

86ELK/ARM Elkind, J. L., Armentrout, P. B., "Transition-metal hydride bond energies: first and second row", Inorg. Chem., 25(8), 1078-1080 (1986), CA104(20):177178f, enthalpy of formation

86KOL/GAG Kolbanovskii, Yu. A., Gagarin, S. G., "Orbital resonance in gaseous reactions between metal monohydride ions and methane", Izv. Akad. Nauk SSSR, Ser. Khim., (6), 1291-1294 (1986), CA105(14):121181e, ionization potential

86SCH/GOD Schilling, J. B., Goddard, W.A., III, Beauchamp, J. L., "Theoretical studies of transition-metal hydrides. 1. Bond energies for MH^+ with M = Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn", J. Am. Chem. Soc., 108(4), 582-584 (1986), CA104(12):95921d, dissociation energies

87MIL/FEI Miller, A.E.S., Feigerle, C.S., Lineberger, W.C., "Laser photoelectron spectroscopy of CrH^-, CoH^-, and NiH^-: periodic trends in the electronic structure of the transition-metal hydrides", J. Chem. Phys., 87(3), 1549-1556 (1987), electron affinity, electronic energy levels, vibrational analysis

74BAR/CER Bartovska, L., Cerny, C., Bartovsky, T., "The study of systems cobalt-iodine and nickel-iodine at higher temperatures", Coll. Czech. Chem. Commun., 39, 917-923 (1974), dissociation energy

38MIE Miescher, E., "Molecular spectra of halides of the iron group, particularly FeCl", Helv. Phys. Acta, 11, 463-468 (1938), emission spectra, may not contain data

39MES Mesnage, P., "Researches on high frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), vibrational analysis, emission spectra, electronic energy levels

59RED Reddy, S.P., "New band systems of FeBr in the visible region", J. Sci. Industr. Res. (India), 18B, 188-190 (1959), CA55:18292a, emission spectra, electronic energy levels, vibrational analysis

70RAO/RAO Rao, N.V.K., Rao, P.T., "New band system of the iron bromide [FeBr] molecule", J. Phys. B, 3(5), 725-728 (1970), CA73(10):50458h, emission spectra, electronic energy levels, vibrational analysis

74BRI/CAL Brinton, R.K., Callear, A.B., "Chemical rearrangement in the reaction of iron(1+) ion with hexafluorosulfate(1-) ion. New spectra of iron halides", J. Chem. Soc., Faraday Trans. 2, 70(2), 203-214 (1974), CA81(2):6581j, emission spectra, electronic energy levels

86KHA/GER Kharitonov, Yu.Ya., Gerzha, T.V., Averbukh, B.S., Kuznetsov, S.L., "Thermodynamic properties of gaseous di-and monohalides of iron, cobalt and nickel", Zh. Neorg. Khim., 31(7), 1679-1682 (1986), CA105(14):121784d, Eng. transl., Russ. J. Inorg. Chem., 31(7), 961-963 (1986), thermodynamic properties

35MES Mesnage, P., "Molecular emission spectra of some metallic salts", Compt. Rend., 201, 389-391 (1935), CA29:6503(2), emission spectra, electronic energy levels

37SCH/GER Schmid, R., Gero, L., "The limit curve of dissociation on the basis of band spectroscopy", Z. Physik, 104, 724-734 (1937), CA31:4898(8), dissociation energy

38MIE Miescher, E., "Molecular spectra of halogens of the iron group, particularly FeCl", Helv. Phys. Acta, 11, 463-468 (1938), emission spectra, electronic energy levels, vibrational analysis

39MES Mesnage, P., "Researches on high frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), vibrational analysis, emission spectra, electronic energy levels

43MUE Mueller, W., "High multiplicity terms in molecular spectra", Helv. Phys. Acta, 16, 3-32 (1943), CA38:5143(6), emission spectra, vibrational analysis, electronic energy levels

57ALL Allen, T.L., "Bond energies of transition metal halides", J. Chem. Phys., 26(6), 1644-1647 (1957), CA51:17278f, dissociation energy

59SCH/ETZ Schaeffer, H., Etzel, K., "On the transport of the metals iron and nickel with the reactions Me + HCl = $MeCl_2(g) + H_2$ and on the stability of the gas forming subchlorides FeCl and NiCl", Z. Anorg. Allg. Chem., 301, 137-153 (1959), CA54:2896, enthalpy of formation

60RED/RAO Reddy, S.P., Rao, P.T., "The spectrum of iron monochloride in the visible", J. Mol. Spectrosc., 4, 16-22 (1960), CA55:13045e, emission spectra, electronic energy levels, vibrational analysis

69KAN/MCC Kana'an, A.S., McCreary, J.R., Peterson, D.E., Thorn, R.J., "Enthalpy and entropy of sublimation of ferrous chloride; thermochemical properties of gaseous $FeCl_2$", High Temp. Sci., 1(2), 222-231 (1969), CA71(22):105973p, dissociation energy

69RAO Rao, P.T., "High multiplicity electronic transitions in molecular spectra", Bhagavantam Vol. Ed: Balakrishna, S., Bangalore Printing and Publ. Co., Ltd., Bangalore, India, 18-21 (1969), CA73(10):50323k, electronic energy levels

69RAO/RAO Rao, D.V.K., Rao, P.T., "High multiplicity electronic transitions in the spectrum of FeCl", Curr. Sci., 38, 87 (1969), emission spectra, vibrational analysis, electronic energy levels

70RAO/RAO Rao, N.V.K., Rao, D.V.K., Rao, P.T., "Spectrum of iron chloride (FeCl) in the red", Curr. Sci., 39(17), 392-393 (1970), CA73(22):114686r, emission spectra

70RAO/RAO2 Rao, D.V.K., Rao, P.T., "Isotope shift studies and multiplet analysis of system I of iron chloride", J. Phys. B, 3(6), 878-881 (1970), CA73(6):30322f, electronic energy levels

71RAO/RAO Rao, D.V.K., Rao, P.T., "Complex band spectrum of FeCl in the ultraviolet region", Indian J. Pure Appl. Phys., 9, 102-105 (1971), CA75:55868t, emission spectra, vibrational analysis, electronic energy levels

74BRI/CAL Brinton, R.K., Callear, A.B., "Chemical rearrangement in the reaction of iron(1+) ion with hexafluorosulfate(1-) ion. New spectra of iron halides", J. Chem. Soc., Faraday Trans 2, 70(2), 203-214 (1974), CA81(2):6581j, emission spectra, electronic energy levels

76BOR Borisov, Yu.A., "The virial-statistical method for calculating the energies of atoms and molecules. II. Energies and atomization of molecules", Zh. Strukt. Khim., 17(6), 979-984 (1976), CA86(18):128442p, Eng. transl., J. Struct. Chem., 17, 839-843 (1976), dissociation energy

80DAI Daidoji, H., "Spectral interferences in atomic absorption spectrometry. IX. Molecular absorption spectra of beryllium, cerium, lanthanum, iron, and platinum salts", Bunko Kenkyu, 29(5), 326-331 (1980), CA94(14):113721v, absorption spectra

80DEL/DUF Delaval, J.M., Dufour, C., Schamps, J., "Rotational analysis of ultraviolet systems of iron monochloride radical", J. Phys. B, 13(24), 4757-4769 (1980), CA94(16):129654m, emission spectra, electronic energy levels, rotational analysis

82DEL/SCH Delaval, J.M., Schamps, J., "Interactions between the sextet states of iron monochloride", J. Phys. B, 15(22), 4137-4149 (1982), CA98(14):115926x, electronic energy levels

84SAU/TAT Sauval, A.J., Tatum, J.B., "A set of partition functions and equilibrium constants for 300 diatomic molecules of astrophysical interest", Astrophys. J., Suppl. Ser., 56(2), 193-209 (1984), CA101(22):200866c, thermodynamic properties

86RYZ/KHO Ryzhov, M.Yu., Khodeev, Yu.S., "High temperature thermodynamic study with the help of a quadrupole mass-spectrometer. Enthalpy of formation of monofluorides, monochlorides, difluorides, and dichlorides of iron and nickel in the gas phase", Eleventh All-Union Conference on Calorimetry and Chemical Thermodynamics, Novosibirsk, Part 1, 132-133 (1986), dissociation energy

34HOW/ROC Howell, H.G., Rochester, G.D., "New diatomic band spectra", Proc. Univ. Durham Phil. Soc., 9, 126-134 (1934), CA29:4673(1), spectra

70BAR/CAR Barrow, R.F., Carroll, P.K., (1970), unpublished, cited in 'Spectroscopic Data Relative to Diatomic Molecules', B. Rosen (editor), Pergamon Press, 1970

70SEN/BAR Senior, M., Barrow, R.F., (1970), unpublished, cited in 'Spectroscopic Data Relative to Diatomic Molecules', B. Rosen (editor Pergamon Press, 1970

73RIC/BEA Rice, W.W., Beattie, W.H., "Metal atom oxidation lasers", Chem. Phys. Lett., 19(1), 82-85 (1973), CA78(20):130369y, spectra

74BRI/CAL Brinton, R.K., Callear, A.B., "Chemical rearrangement in the reaction of iron(1+) ion with hexafluorosulfate(1-) ion. New spectra of iron halides", J. Chem. Soc., Faraday Trans. 2, 70(2), 203-214 (1974), CA81(2):6581j, emission spectra

75MAC Macheteau, Y., "Growth of iron crystals by thermal decomposition of gaseous iron fluorides", J. Cryst. Growth, 28(1), 93-102 (1975), CA82(12):78896j, formation

78DEV/VAN DeVore, T.C., Van Zee, R.J., Weltner, W., Jr., "An investigation of the first row transition - metal fluoride molecules using ESR spectroscopy", Proc. - Electrochem. Soc., (Proc. Symp. High Temp. Met. Halide Chem., 1977), 78-1, 187-198 (1978), CA89(14):120290d, electronic energy levels

78POU/SCH Pouilly, B., Schamps, J., Lumley, D.J.W., Barrow, R.F., "Electronic states of the iron fluoride (FeF) molecule. I. Analysis of rotational structure", J. Phys. B, 11(13), 2281-2287 (1978), CA90(6):46128j, emission spectra, electronic energy levels, rotational analysis

78POU/SCH2 Pouilly, B., Schamps, J., Lumley, D.J.W., Barrow, R.F., "Electronic states of the iron fluoride (FeF) molecule. II. Ab initio calculations", J. Phys. B, 11(13), 2289-2299 (1978), CA90(6):46129k, electronic energy levels, emission spectra

79THA/SAN Thakur, L., Sandwar, B.B., "Cohesive energies and the relative stabilities of the first row transition metal fluorides", J. Indian Chem. Soc., 56(7), 663-665 (1979), CA92(4):29465r, dissociation energy

81SOR/SID Sorokin, I.D., Sidorov, L.N., Nikitin, M.I., Skokan, E.V., "Mass spectrometric determination of the enthalpies of dissociation of gaseous complex fluorides into neutral charged particles. V. Heats of formation of trifluoroferrate (FeF_3^-) and tetrafluoroferrate (FeF_4^-)", Int. J. Mass Spectrom. Ion Phys., 41, 45-54 (1981), enthalpy of formation

82PAT/KOR Patil, V.S., Korwar, V.M., "Franck-Condon factors for iron fluoride (FeF) ($X^6\Delta_{9/2}$-$^6\Pi_{7/2}$) and lutetium deuteride (LuD) ($X^1\Sigma$-$H^1\Pi$) transitions", Acta Cienc. Indica, [Ser.] Phys., 8(1-4), 7-8 (1982), CA98(18):151898y, spectra

84GOR/MIL Gorokhov, L.N., Milushin, M.I., Ryzhov, M.Yu., Smirnov, V.K., Khodeev, Yu.S., Chekhovskoi, D.V., "Problems in mass-spectrometric studies of high-temperature equilibria and enthalpies of formation of iron fluoride (FeF), lead fluoride (PbF_2), lead fluoride (PbF), and uranium fluoride (UF_5) molecules", Probl. Kalorim. Khim. Termodin., Dokl. Vses. Konf., 10th, Ed.: Emanuel, I.M., 2, 463-465 (1984), CA104(6):40742r, enthalpy of formation

84SAU/TAT Sauval, A.J., Tatum, J.B., "A set of partition functions and equilibrium constants for 300 diatomic molecules of astrophysical interest", Astrophys. J., Suppl. Ser., 56(2), 193-209 (1984), CA101(22):200866c, thermodynamic properties

85GOR/RYZ Gorokhov, L.N., Ryzhov, M.Yu., Khodeev, Yu.S., "Heats of formation of gaseous iron and magnesium fluorides (FeF, FeF_2, MgF)", Zh. Fiz. Khim., 59(12), 2939-2943 (1985), CA104(8):57202n, Eng. transl., Russ. J. Phys. Chem., 59, 1761-1764 (1985), enthalpy of formation

86RYZ/KHO Ryzhov, M.Yu., Khodeev, Yu.S., "High temperature thermodynamic study with the help of a quadrupole mass-spectrometer. Enthalpy of formation of monofluorides, difluorides, and dichlorides of iron and nickel in the gas phase", Eleventh All-Union Conference on Calorimetry and Chemical Thermodynamics, Novosibirsk, Part 1, 132-133 (1986), dissociation energy

26WEI Weichselfelder, T., "Hydrides of the metals nickel, cobalt, iron and chromium", Annalen der Chemie, Justus Liebigs, 447, 64-77 (1926), CA20:1363, spectra, with Thiede, B.;

29FRA/MAY Frankenburg, W., Mayrhofer, K., "Atomized iron", Z. Elektrochem., 35, 590-600 (1929), CA24:2026, spectra

36HEI Heimer, A., "The band spectrum of FeH", Naturwissenschaften, 24, 492 (1936), CA31:33(5), spectra

46RAY/SAH Ray, R.C., Sahai, R.B.N., "Hydrides of iron", J. Indian Chem. Soc., 57-72 (1946), CA40:7034, spectra

65MUK/MUK Mukhtarov, I.A., Mukhtarov, R.I., "Centrifugal perturbation constants of the 1,1,2-trifluoroethane molecules", Optika i Spektroskopiya, 19(6), 979-980 (1965), CA64:18677e, Eng. transl., Opt. Spectrosc., 19, 546 (1965), enthalpy of formation

67MCD/BRO McDugle, W.G., Jr., Brown, T.L., "A new evaluation of Platt's model for diatomic hydrides", J. Am. Chem. Soc., 89(13), 3111-3114 (1967), CA67(10):47295y, bond length

72CAR/MCC Carroll, P.K., McCormack, P., "Spectrum of iron hydride. Laboratory and solar identification", Astrophys. J., 177(1), Pt. 2, L33-L36 (1972), CA77(26):171088d, visible spectra

72MAS Mastryukov, V.S., "Nucleus-nucleus distances in diatomic hydrides", Zh. Strukt. Khim., 13(3), 379-383 (1972), CA77(18):118372r, Eng. transl., J. Struct. Chem., 13, 359-362 (1972), bond distance

72WAL/WAL Walker, J.H., Walker, T.E.H., Kelly, H.P., "Ground and low-lying excited electronic states of iron monohydride", J. Chem. Phys., 57(5), 2094-2098 (1972), CA77(20):132603y, electronic energy levels

73SMI Smith, R.E., "Diatomic hydride and deuteride spectra of the second row transition metals", Proc. Roy. Soc. London, Ser. A, 332(1588), 113-127 (1973), CA78(12):77638g, absorption spectra, electronic energy levels, vibrational analysis

74SCO Scott, J.E., Jr., "Atomic interactions basic to macroscopic properties of gases", U. S., Aerosp. Res. Lab., Report, ARL-TR-74-0103, 102pp (1974), CA82(16):103278u, dissociation energy

75SCO/RIC Scott, P.R., Richards, W.G., "Electronic structure of iron hydride (FeH)", J. Chem. Phys., 63(4), 1690-1691 (1975), CA83(18):154845e, electronic structure

76CAR/MCC Carroll, P.K., McCormack, P., O'Connor, S., "Iron hydride: laboratory studies and solar identification", Astrophys. J., 208(3, Pt. 1), 903-913 (1976), CA85(18):133973w, spectra

76MCC/O'C McCormack, P., O'Connor, S., "Wavelengths and line intensities for the 4920 P, 5320 P and 8690 P bands of iron hydride (FeH)", Astron. Astrophys., Suppl. Ser., 26(3), 373-380 (1976), CA86(14):98398j, visible spectra

77MID Middleton, R., "A survey of negative ions from a cesium sputter source", Nucl. Instrum. Methods, 144(3), 373-399 (1977), CA87(24):190803f, formation

77TAR Tarafdar, S.P., "Partition functions and equilibrium constants of some positive molecular ions", J. Quant. Spectrosc. Radiat. Transfer, 17(4), 537-542 (1977), CA86(24):179681y, partition function

78GEL Gelatt, C.D., "Calculated heats of formation of metal and metal alloy hydrides", Hydrides Energy Storage, Proc. Int. Symp., 1977, Eds: Andresen, A.F., Maeland, A.J., Pergamon, Oxford, England, 193-204 (1978), CA91(8):63504s, enthalpy of formation

78GEL/EHR Gelatt, C.D., Jr., Ehrenreich, H., Weiss, J.A., "Transition-metal hydrides: Electronic structure and the heats of formation", Phys. Rev. B, 17(4), 1940-1957 (1978), CA88(26):197793g, enthalpy of formation

79ALT/BLA Alton, G.D., Blazey, G.C., "Studies associated with the development of a modified University of Aarhus negative ion source", Nucl. Instrum. Methods, 166(2), 105-116 (1979), CA92(6):48932g, formation

79DEN/VAN Dendramis, A., Van Zee, R.J., Weltner, W., Jr., "The iron hydride (FeH) molecule at 4 K", Astrophys. J., 231(2, Pt.1), 632-636 (1979), CA91(14):114813b, matrix isolation spectra

79DIX/ROB Dixon, R.N., Robertson, I.L., "A comparison of semilocal and nonlocal pseudopotential techniques calculations on iron and iron monohydride cation", Mol. Phys., 37(4), 1223-1237 (1979), CA91(24):199159r, dissociation energy

80BAR/LIT Bar-Nun, A., Litman, M., Pasternak, M., Rappaport, M.L., "The formation of hydrocarbons and iron-hydrides on cold interstellar grains-experimental studies", Symp. - Int. Astron. Union, (Interstellar Mol.), 87, 367-371 (1980), CA94(14):112257m, hydrogen reaction

80BOU/MIE Bouten, P.C.P., Miedema, A.R., "On the heats of formation of the binary hydrides of transition metals", J. Less-Common Met., 71(1), 147-160 (1980), CA93(10):102263a, enthalpy of formation

80KHA/KRA Kharitonov, Yu.Ya., Kravtsova, G.V., "Empirical dependences between force constants and bond length for iron, cobalt, and nickel hydrides", Zh. Neorg. Khim., 25(11), 3053-3058 (1980), CA94(12):92726h, Eng. transl., Russ. J. Inorg. Chem., 25, 1676-1679 (1980), force constant, bond length

81ARM/HAL Armentrout, P.B., Halle, L.F., Beauchamp, J.L., "Periodic trends in transition metal-hydrogen, metal-carbon, and metal-oxygen bond dissociation energies. Correlation with reactivity and electronic structure", J. Am. Chem. Soc., 103(21), 6501-6502 (1981), CA95(18):156742r, ionization potential, dissociation energy

81DAS Das, G., "A pseudopotential study of the iron-series transition metal hydrides", J. Chem. Phys., 74(10), 5766-5774 (1981), CA95(2):13166v, dissociation energy, vibrational analysis

81KAN/MOO Kant, A., Moon, K.A., "Mass spectrometric determination of the dissociation energies of gaseous aluminum hydride, gallium hydride, indium hydride, scandium hydride, and cobalt hydride and estimation of the maximum dissociation energies of thallium hydride, chromium hydride, manganese hydride, and iron hydride", High Temp. Sci., 14(1), 23-31 (1981), CA95(12):103738n, dissociation energy

81KHA/KRA Kharitonov, Yu.Ya., Kravtsova, G.V., "Thermodynamic functions of diatomic hydrides of Group VIII metals", Zh. Neorg. Khim., 26(5), 1198-1201 (1981), CA95(4):31394x, Eng. transl., Russ. J. Inorg. Chem., 26, 645-647 (1981), thermodynamic properties

82SAK/PIC Sakurai, T., Pickering, H.W., "High-performance time-of-flight atom probe for hydrogen characterization in metals", Adv. Tech. Charact. Hydrogen Met., Proc. Symp., 1981, Eds: Fiore, N.F., Berkowitz, B.J., Metall. Soc. AIME, Warrendale, PA, 171-181 (1982), CA98(14):111782z, hydrogen reaction

82SAK/PIC2 Sakurai, T., Pickering, H.W., "High performance time-of-flight atom-probe for characterization of hydrogen in metals", AIP Conf. Proc., (Phys. Steel Ind.), 84, 99-112 (1982), CA98(4):20254n, hydrogen reaction

83BAL/LIN Balfour, W.J., Lindgren, B., O'Connor, S., "Rotational analysis of the 9877 and 8960 Å bands of iron deuteride (FeD)", Phys. Scr., 28(5), 551-560 (1983), CA100(6):42141k, rotational analysis, absorption spectra, emission spectra, electronic energy levels

83BAL/LIN2 Balfour, W.J., Lindgren, B., O'Connor, S., "On the 1 μm system of iron hydride", Chem. Phys. Lett., 96(2), 251-252 (1983), CA98(20):169712t, electronic energy levels, rotational analysis

83CAR/SAL Carlin, T.J., Sallans, L., Cassady, C.J., Jacobson, D.B., Freiser, B.S., "Gas-phase reactions of Group VIII metal hydride ions (FeD^+, CoD^+, and NiD^+) with hydrocarbons", J. Am. Chem. Soc., 105(2), 6320-6321 (1983), CA99(17):140141r, ionization potential

83STE/FEI Stevens, A.E., Feigerle, C.S., Lineberger, W.C., "Laser photoelectron spectroscopy of manganese hydride (MnH^-) and iron hydride (FeH^-): electronic structures of the metal hydrides, identification of a low-spin excited state of manganese hydride (MnH), and evidence for a low-spin ground state of iron hydride (FeH)", J. Chem. Phys., 78(9), 5420-5431 (1983), CA99(4):30261x, electron affinity, electronic energy level

83WAL/BAU Walch, S.P., Bauschlicher, C.W., Jr., "CASSCF/CI calculations for first row transition metal hydrides: The titanium hydride (TiH)($^4\Phi$), vanadium hydride (VH)($^5\Delta$), chromium hydride (CrH)($^6\Sigma^+$), manganese hydride (MnH)($^7\Sigma^+$), iron hydride (FeH)($^{4,6}\Delta$), and nickel hydride (NiH)($^2\Delta$) states", J. Chem. Phys., 78(7), 4597-4605 (1983), CA98(20):167166u, electronic energy level

84HAL/KLE Halle, L.F., Klein, F.S., Beauchamp, J.L., "Properties and reactions of organometallic fragments in the gas phase. Ion beam studies of hydridoiron(1+) ion", J. Am. Chem. Soc., 106(9), 2543-2549 (1984), CA100(25):210081m, dissociation energy

84MAN/HAL Mandich, M.L., Halle, L.F., Beauchamp, J.L., "Determination of the metal-hydrogen and metal-methyl bond dissociation energies of the second-row, Group 8 transition metal cations", J. Am. Chem. Soc., 106(16), 4403-4411 (1984), CA101(9):72937n, dissociation energy

84PAS/VAN Pasternak, M., Van der Heyden, M., Langouche, G., "The characterization of iron hydride (FeH) molecules by Moessbauer spectroscopy", Chem. Phys. Lett., 104(4), 398-400 (1984), CA100(18):148027t, Moessbauer spectroscopy

84WAL Walch, S.P., "Theoretical evidence supporting the $^4\Delta$ ground-state assignment for iron hydride (FeH)", Chem. Phys. Lett., 105(1), 54-57 (1984), CA100(18):145197n, electronic energy level

84WIN Winkel, R.J., "Infrared spectra of diatomic molecules of astrophysical interest - carbon monosulfide, sulfur monohydride, iron hydride", Dissertation, 192pp (1984), CA104(12):98471t, spectra, available Univ. Microfilms Int., Order No. DA8513044 from Diss. Abstr. Int. B 1985, 46(4), 1216

85SAL/LAN Sallans, L., Lane, K.R., Squires, R.R., Freiser, B.S., "Generation and reaction of atomic metal anions in the gas phase. Determination of the heterolytic and homolytic bond energies for the vanadium, chromium, iron, cobalt, and molybdenum hydrides VH, CrH, FeH, CoH, and MoH", J. Am. Chem. Soc., 107(15), 4379-4385 (1985), CA103(6):42997f, dissociation energy

86ALT/BEC Alton, G.D., Beckers, R.M., Johnson, J.W., "A radial geometry cesium plasma source with improved mechanical features", Nucl. Instrum. Methods Phys. Res., Sect. A, A244(1-2), 148-154 (1986), CA104(16):137548v, negative formation

JANAF THERMOCHEMICAL TABLES - IRON BIBLIOGRAPHIES
IRON HYDRIDE (FeH, FeH^+, FeH^-)

86CHI/LAN Chiong, D.P., Langhoff, S.R., Bauschlicher, C.W., Jr., Walch, S.P., Partridge, H., "Theoretical dipole moments for the first-row transition metal hydrides", J. Chem. Phys., 85(5), 2850-2860 (1986), CA105(18):163141x, dipole moment

86ELK/ARM Elkind, J.L., Armentrout, P.B., "Transition-metal hydride bond energies: first and second row", Inorg. Chem., 25(8), 1078-1080 (1986), CA104(20):177178f, dissociation energy

86KOL/GAG Kolbanovskii, Yu.A., Gagarin, S.G., "Orbital resonance in gaseous reactions between metal monohydride ions and methane", Izv. Akad. Nauk SSSR, Ser. Khim., (6), 1291-1294 (1986), CA105(14):121181e, ionization potential

86SCH/GOD Schilling, J.B., Goddard, W.A., III, Beauchamp, J.L., "Theoretical studies of transition-metal hydrides. 1. Bond energies for MH^+ with M = Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn", J. Am. Chem. Soc., 108(4), 582-584 (1986), CA104(12):95921d, dissociation energy

87DOL/WED Dolg, M., Wedig, U., Stoll, H., Preuss, H., "Ab initio pseudopotential study of the first row transition metal monoxides and iron monohydride", J. Chem. Phys., 86(4), 2123-2131 (1987), CA106(24):202095c, electronic ground state

84GRA/ROS Grade, M., Rosinger, W., Dowben, P.A., "Core and valence electron binding energies of iron(II) iodide and stabilities of gas phase species", Ber. Bunsen-Ges. Phys. Chem., 88(1), 65-71 (1984), CA100(10):74331p, ionization potential, dissociation energy

85GRA/ROS Grade, M., Rosinger, W., "Correlation of electronic structures and stabilities of gaseous FeI_2, Fe_2I_2 and Fe_2I_4 molecules, solid [FeI_2], and iodine absorbed on [Fe]", Surface Sci., 156, 920-929 (1985), CA103(10):76670j, ionization potential, electronic structure

85HIL/VIS Hilpert, K., Viswanathan, R., Gingerich, K.A., Gerads, H., Kobertz, D., "Vaporization of FeI_2(s) and the thermochemistry of FeI_2(g), $(FeI_2)_2$(g), $(FeI_2)_3$(g), and FeI_3(g)", J. Chem. Thermodyn., 17(5), 423-436 (1985), CA103(4):28216u, appearance potential

37MES Mesnage, P., "Molecular emission spectra of some metallic salts", Compt. Rend., 204, 1929-1931 (1937), CA31:6108(8), emission spectra, electronic energy levels

39MES Mesnage, P., "Researches on high-frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), emission spectra, vibrational analysis, electronic energy levels

52KRI Krishnamurty, V.G., "Complex band spectrum of nickel bromide", Curr. Sci. (India), 21, 98 (1952), CA46:10879i, emission spectrum, vibrational analysis, electronic energy levels, See also CA51:7850c

52KRI2 Krishnamurty, V.G., "The complex band spectrum of nickel bromide", Indian J. Phys., 26, 429-441 (1952), CA51:7850c, vibrational analysis, emission spectra, electronic energy levels, See also CA46:10879i

60RED/RAO Reddy, S.P., Rao, P.T., "The band spectra of NiCl and NiBr in the visible", Proc. Phys. Soc., (London), 75, [Pt.2], 275-279 (1960), CA54:17040a, vibrational analysis, emission spectra, electronic energy levels

61BUL/PHI Bulewicz, E.M., Phillips, L.F., Sugden, T.M., "Determination of dissociation constants and heats of formation of molecules by flame photometry. VIII. Stabilities of the gaseous diatomic halides of certain metals", Trans. Faraday Soc., 57, 921-931 (1961), CA56:73f, dissociation energy

62SUN Sundarachary, N., "Emission spectrum of NiBr", Proc. Natl. Acad. Sci., India Sect. A, 32[3], 311-319 (1962), CA58:10863f, emission spectrum

64MCK McKinley, J.D., "Mass spectrometric investigation of the nickel-bromine surface reaction", J. Chem. Phys., 40(2), 576-581 (1964), CA60:3709g, formation

79DAR/SHA Darji, A. B., Shah, N. R., "New band system of nickel(I) bromide molecule in the near ultraviolet region", Curr. Sci., 48(18), 809-810 (1979), CA91(24):201532c, vibrational analysis, emission spectra, electronic energy levels

80GOP/JOS Gopal, R., Joshi, M. M., "New band systems of nickel bromide molecule in visible region", Pramana, 15(4), 349-356 (1980), CA94(2):9512s, emission spectra, electronic energy levels, vibrational analysis

81GOP/JOS Gopal, R., Joshi, M. M., "Thermal emission spectrum of H → X and I → X systems of nickel bromide molecule", Curr. Sci., 50(24), 1061-1063 (1981), CA96(8):60290m, emission spectrum, vibrational analysis, electronic energy levels

82BOE/SCH Boehm, M. C., Schmidt, P. C., Sen, K. D., "Molecular orbital electronegativities of transition metal fragments: a MO approach based on the transition operator method", THEOCHEM, 4(1), 43-52 (1982), CA96(22):187490g, electron affinity

82GOP/JOS Gopal, R., Joshi, M. M., "Thermal emission spectrum of nickel monobromide molecule in the region λλ4845-4300 P", Indian J. Pure Appl. Phys., 20(9), 763-764 (1982), CA98(4):24931d, vibrational analysis, emission spectra, electronic energy levels

85GOP/JOS Gopal, R., Joshi, M. M., "Vibrational analysis of violet spectrum of nickel bromide (NiBr) molecule", Indian J. Phys., B, 59B(4), 309-312 (1985), CA103(18):149933j, vibrational analysis, emission spectra, electronic energy levels

86KHA/GER Kharitonov, Yu. Ya., Gerzha, T. V., Averbukh, B. S., Kuznetsov, S. L., "Thermodynamic properties of gaseous di-and monohalides of iron, cobalt and nickel", Zh. Neorg. Khim., 31(7), 1679-1683 (1986), CA105(14):121784d, Eng. transl., Russ. J. Inorg. Chem., 31(7), 961-963 (1986), thermodynamic properties

37MOR More, K.R., "Band spectra of NiCl and CoCl", Phys. Rev., 51, 1019 (1937), CA32:5294(4), emission spectra, vibrational analysis, electronic energy levels

38MIE Miescher, E., "Molecular spectra of halogens of the ion group, particularly FeCl", Helv. Phys. Acta, 11, 463-468 (1938), emission spectra

38MOR More, K.R., "Spectra of the monochlorides of nickel, cobalt and iron", Phys. Rev., 54, 122-125 (1938), CA32:7342(9), emission spectrum, vibrational analysis, electronic energy levels

39MES Mesnage, P., "Researches on high-frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), vibrational analysis, emission spectra, electronic energy levels

52KRI Krishnamurty, V.G., "The complex band spectrum of nickel chloride", Indian J. Phys., 26, 207-225 (1952), CA47:1487c, emission spectra, vibrational analysis, electronic energy levels, See also CA46:10879h

52KRI2 Krishnamurty, V.G., "Complex band spectrum of nickel chloride", Curr. Sci. (India), 21, 66 (1952), CA46:10879h, emission spectra, vibrational analysis, electronic energy levels, see also CA47:1487c

56SCH/BRE Schafer, V.H., Breil, G., "Uber die neigung zur bildung gasformiger trichloride bei den elementen Cr, Mn, Fe, Co, Ni, untersuchmit der reaktion $MeCl_2$gas + $1/2Cl_2$ = $MeCl_3$gas", Z. Anorg. Allg. Chem., 283, 304-313 (1956), enthalpy of formation

57ALL Allen, T., "Bond energies of transition metal halides", J. Chem. Phys., 26(6), 1644-1647 (1957), CA51:17278, dissociation energy

59SCH/ETZ Schafer, H., Etzel, K., "Chemical transport reactions. VI. The transport of metallic iron and nickel by the reaction M + 2HCl = MCl_2 and NiCl", Z. Anorg. Allg. Chem., 301, 137-153 (1959), CA54:2896g, enthalpy of formation

60RED/RAO Reddy, S.P., Rao, P.T., "The band spectra of NiCl and NiBr in the visible", Proc. Phys. Soc. (London), 75, 275-279 (1960), CA54:17040a, emission spectra, vibrational analysis, electronic energy levels

61BUL/PHI Bulewicz, E.M., Phillips, L.F., Sugden, T.M., "Determination of dissociation constants and heats of formation of molecules by flame photometry. VIII. Stabilities of the gaseous diatomic halides of certain metals", Trans. Faraday Soc., 57, 921-931 (1961), CA56:73f, dissociation energy

62MCK McKinley, J.D., "Transitional energy accomodation in the nickel-chlorine surface reaction", J. Phys. Chem., 66(3), 554-556 (1962), CA56:12351e, formation

62RAO/RED Rao, S.V.K., Reddy, S.P., Rao, P.T., "New band systems of NiCl in the photographic infrared", Z. Physik, 166, 261-264 (1962), CA56:8174d, emission spectra, vibrational analysis, electronic energy levels

63SMI/FIT Smith, J.N., Jr., Fite, W.L., "Gas-surface interactions using modulated-atomic-beam techniques", Proc. Intern. Symp. Rarefied Gas Dyn., 1, 430-453 (1963), CA62:3419f, enthalpy of formation

64MCK McKinley, J.D., "Mass-spectrometric investigation of the high-temperature reaction between nickel and chlorine", J. Chem. Phys., 40, 120-125 (1964), CA60:2356a, appearance potential

65STA/GUI Stahel, E., Guillissen, J., "Spectra of matrix-isolated NiF_2 and $NiCl_2$", J. Chem. Phys., 42(3), 902-905 (1965), discussion of Miescher article

69RAO/RAO Rao, N. V. K., Rao, P. T., "Emission spectrum of nickel monochloride", Curr. Sci., 38(24), 589-590 (1969), CA72(10):49329q, emission spectra, vibrational analysis, electronic energy levels, rotational analysis

71RAO/DAD Rao, B. S., Dadape, V. V., "Sublimation pressure of nickel dichloride and the study of the reaction $Ni(c)+NiCl_2(g)=2NiCl(g)$", High Temp. Sci., 3(1), 1-9 (1971), CA75(2):11175k, enthalpy of formation

76WIE Wiedijk, P., "Simultaneous microdetermination of water and oxygen in metal halides by reductive fusion in an inert gas", Anal. Chim. Acta, 81(1), 105-110 (1976), CA85(4):28210x, formation

80DAR/SHA Darji, A. B., Shah, N. R., "New spectrum of nickel chloride (NiCl) molecule in the near ultraviolet region", Indian J. Pure Appl. Phys., 18(10), 802-805 (1980), CA93(24):227962j, emission spectra, vibrational analysis, electronic energy levels

81GOP Gopal, R., "Thermal emission spectrum of B → X system of nickel chloride (NiCl) molecule", Curr. Sci., 50(19), 854-855 (1981), CA95(24):212367m, emission spectra, vibrational analysis, electronic energy levels

81GOP/JOS Gopal, R., Joshi, M. M., "New band systems of nickel monochloride molecule", Indian J. Phys., [Part] B, 55B(5), 368-376 (1981), CA96(4):26534j, emission spectra, vibrational analysis, electronic energy levels

82BOE/SCH Boehm, M. C., Schmidt, P. C., Sen, K. D., "Molecular orbital electronegativities of transition metal fragments: a MO approach based on the transition operator method", THEOCHEM, 4(1), 43-52 (1982), CA96(22):187490g, electron affinity

82GOP/JOS Gopal, R., Joshi, M. M., "Thermal emission spectrum of the nickel monochloride molecule in λλ4730-4390 P region", Indian J. Pure Appl. Phys., 20(4), 280-283 (1982), CA97(2):14385u, emission spectra, vibrational analysis, electronic energy levels

83GOP/JOS Gopal, R., Joshi, M. M., "Thermal emission spectrum of nickel monochloride molecule in violet region", Indian J. Pure Appl. Phys., 21(10), 595-598 (1983), CA100(6):42117g, emission spectra, vibrational analysis, electronic energy levels

83SHA/DAR Shah, P. M., Darji, A. B., Shah, N. R., "New spectrum of nickel monochloride molecule", Indian J. Pure Appl. Phys., 21(10), 617-618 (1983), CA100(6):42203g, emission spectra, vibrational analysis, electronic energy levels

86RYZ/KHO Ryzhov, M.Yu., Khodeev, Yu.S., "High temperature thermodynamic study with the help of a quadrupole mass-spectrometer. Enthalpy of formation of monofluorides, monochlorides, difluorides, and dichlorides of iron and nickel in the gas phase", Eleventh All-Union Conference on Calorimetry and Chemical Thermodynamics, Novosibirsk, Part 1, 132-133 (1986), dissociation energy

53KRI Krishnamurty, V.G., "The band spectrum of nickel fluoride", Indian J. Phys., 27, 354-358 (1953), CA51:7850b, emission spectra, electronic energy levels, vibrational analysis

64BAL/MOC Balkanski, M., Moch, P., Parisot, G., "Infrared spectra of lattice vibrations of nickel fluorides", Compt. Rend., 258, 2785-2787 (1964), CA63:153f, infrared spectra

64EHL/KEN Ehlert, T.C., Kent, R.A., Margrave, J.L., "Mass-spectrometric studies at high temperatures. VI. The sublimation pressure of nickel(II) fluoride", J. Am. Chem. Soc., 86, 5093-5095 (1964), CA62:2261f, enthalpy of formation

66MCK McKinley, J.D., "Mass-spectrometric investigation of the nickel-fluorine surface reaction", J. Chem. Phys., 45(5), 1690-1693 (1966), CA65:12984a, formation

66POL Polyachenok, O. G., "Dissociation energy of diatomic halide molecules", Zh. Fiz. Khim., 40(10), 2644-2647 (1966), CA66(6):22846v, Eng. transl., Russ. J. Phys. Chem., 40, 1420-1422 (1966), dissociation energy

71MOV/KUZ Movchan, B. A., Kuz'min, G. S., Mochalova, T. F., Karatysh, V. V., Tikhonovskii, A. L., Yagupol'skaya, L. N., "Corrosion of nickel of varying purity in gaseous hydrogen fluoride", Zashch. Metal., 7(1), 32-34 (1971), CA74(16):78875m, Eng. transl., Protection of Metals, 7, 22-23 (1971), formation

73RIC/BEA Rice, W. W., Beattie, W. H., "Metal atom oxidation lasers", Chem. Phys. Lett., 19(1), 82-85 (1973), CA78(20):130369y, emission spectra, formation

78DEV/VAN DeVore, T. C., Van Zee, R. J., Weltner, W., Jr., "An investigation of the first row transition - metal fluoride molecules using ESR spectroscopy", Proc. - Electrochem. Soc., Proc. Symp. High Temp. Met. Halide Chem., 1977, 78-1, 187-198 (1978), CA89(14):120290d, ground state, electronic configuration

79PIN/LEF Pinchemel, B., Schamps, J., "Rotational analysis of a $^2\Delta$-$^2\Pi$ system of nickel fluoride (NiF)", J. Mol. Spectrosc., 77(1), 29-35 (1979), CA91(6):46807a, rotational analysis, electronic energy levels, emision spectra

81GOP/JOS Gopal, R., Joshi, M. M., "New band systems of the nickel fluoride (NiF) molecule", Curr. Sci., 50(12), 530-531 (1981), CA95(8):70367k, vibrational analysis, emission spectra, electronic energy levels

81GOP/SIN Gopal, R., Singh, L. K., Joshi, M. M., "Thermal emission spectrum of H → X and I → X systems of nickel(I) fluoride molecule", Indian J. Phys., [Part] B, 55B(6), 507-509 (1981), CA96(16):132536w, emission spectra, vibrational analysis, electronic energy levels

81PIN Pinchemel, B., "Rotational analysis of a $B^2\Pi$-$X^2\Sigma^+$ transition of nickel monofluoride", J. Phys. B, 14(15), 2569-2573 (1981), CA95(26):228311z, rotational analysis, electronic energy levels, emission spectra

84SAU/TAT Sauval, A. J., Tatum, J. B., "A set of partition functions and equilibrium constants for 300 diatomic molecules of astrophysical interest", Astrophys. J., Suppl. Ser., 56(2), 193-209 (1984), CA101(22):200866c, thermodynamic properties

86BAI/HIL Bai, J., Hilborn, R.C., "Chemiluminescence and laser-induced fluorescence of nickel fluoride (NiF)", Chem. Phys. Lett., 128(2), 133-136 (1986), CA105(12):105044g, electronic energy levels, chemiluminescence, fluorescence

86RYZ/KHO Ryzhov, M.Yu., Khodeev, Yu.S., "High temperature thermodynamic study with the help of a quadrupole mass-spectrometer. Enthalpy of formation of monofluorides, monochlorides, difluorides, and dichlorides of iron and nickel in the gas phase", Eleventh All-Union Conference on Calorimetry and Chemical Thermodynamics, Novosibirsk, Part 1, 132-133 (1986), dissociation energy

34GAY/PEA Gaydon, A.G., Pearse, R.W.B., "Spectrum of nickel hydride", Nature, 134, 287 (1934), CA28:7155(9), spectra

35GAY/PEA Gaydon, A.G., Pearse, R.W.B., "Band spectrum of nickel hydride: Bands at λ5713, λ6246, and λ6424", Proc. Roy Soc. A (London), A148, 312-335 (1935), CA29:2847(5), spectra

36HEI Heimer, A., "Band spectra of NiH and CoH", Naturwissenschaten, 24, 413 (1936), CA31:33(9), spectra

37HEI Heimer, A., "The red band spectrum of nickel hydride", Z. Physik, 105, 56-72 (1937), CA31:5270(3), spectra

37HEI2 Heimer, A., Theses, Stockholm (1937), spectra

46GUG Guggenheimer, K.M., "New regularities in vibrational spectra", Proc. Phys. Soc. (London), 58, 456-468 (1946), CA40:6991, vibrational spectra

59VAR/MIT Varshni, Y.P., Mitra, S.S., Shukla, R.C., "Spectroscopic constants of molecules. VII. Relation between force constant and equilibrium internuclear distance for hydride diatoms", Indian J. Phys., 33, 473-482 (1959), CA54:10496a, bond distance

63AND/LAG Andersen, E., Lagerqvist, A., Neuhas, H., Aslund, N., "Bands of NiH and NiD in the violet region of the spectrum", Proc. Phys. Soc., 82(528), 637-638 (1963), CA59:10897a, emission spectra

64ASL/NEU Aslund, N., Neuhas, H., Lagerqvist, A., Andersen, E., "Rotational analysis of violet bands of NiH and NiD", Arkiv Fysik, 28(24), 271-283 (1964), CA63:10866g, rotational analysis, electronic energy levels

65CAR/CAR Carbo, R., de Carbo, C.A., Molina, J., "Calculation of the energy of the ground state of diatomic molecules by an L.C.A.O.-S.C.F. method", Afinidad, 22(240), 403-405 (1965), CA64:18677e, dissociation energy

66POL Politzer, P., "Bond lengths and atomic orbital radii in the diatomic hydrides", J. Phys. Chem., 70(12), 4041-4044 (1966), CA66(6):22408d, bond lengths

73SMI Smith, R. E., "Diatomic hydride and deuteride spectra of the second row transition metals", Proc. Roy. Soc. London, Ser. A, 332(1588), 113-127 (1973), CA78(12):77638g, absorption spectra, electronic energy levels, vibrational analysis

74SCH Schneider, J., "Internal partial function of two atom molecules in a polynomial representation", Z. Phys. Chem. (Leipzig), 255(5), 986-996 (1974), CA82(22):145259u, thermodynamic properties

77DUN/CON Dunlap, B. I., Connolly, J. W. D., Sabin, J. R., "On the applicability of LCAO-Xα methods to molecules containing transition metal atoms: the nickel atom and nickel hydride", Int. J. Quantum Chem., Symp., Proc. Int. Symp. At., Mol., Solid-State Theory, Collision Phenom., Comput. Methods, 11, 81-87 (1977), CA87(26):206933m, dissociation energy

77GUS/BLI Guse, M. P., Blint, R. J., Kunz, A. B., "Potential energy curves for nickel monohydride and nickel dihydride", Int. J. Quantum Chem., 11(5), 725-732 (1977), CA87(4):29334u, potential energy curve

77MID Middleton, R., "A survey of negative ions from a cesium sputter source", Nucl. Instrum. Methods, 144(3), 373-399 (1977), CA87(24):190803f, formation

78WRI/BAT Wright, R. B., Bates, J. K., Gruen, D. M., "Matrix-isolation spectroscopy of aluminum, copper, and nickel hydrides and deuterides produced in a hollow-cathode discharge", Inorg. Chem., 17(8), 2275-2278 (1978), CA89(12):97307d, vibrational analysis

79KAN/MOO Kant, A., Moon, K.A., "Dissociation energies of gaseous copper, silver, gold, and nickel hydrides", High Temp. Sci., 11(1), 55-62 (1979), CA91(20):163953f, dissociation energy

80ARM/BEA Armentrout, P. B., Beauchamp, J. L., "Endothermic reactions of nickel(1+) ion with diatomic hydrogen, hydrogen deuteride, and diatomic deuterium", Chem. Phys., 50(1), 37-43 (1980), CA93(22):210402d, dissociation energy

80DEV DeVore, T. C., "Rotational analysis of the 502.64 nm band of nickel hydride", High Temp. Sci., 12(4), 259-266 (1980), CA94(18):147881n, rotational analysis

80DUN/YU Dunlap, B. I., Yu, H. L., "An extended basis set LCAO Xα treatment of nickel monohydride and diatomic nickel", Chem. Phys. Lett., 73(3), 525-529 (1980), CA93(14):138260m, dissociation energy

80KHA/KRA Kharitonov, Yu. Ya., Kravtsova, G. V., "Empirical dependences between force constants and bond length for iron, cobalt, and nickel hydrides", Zh. Neorg. Khim., 25(11), 3053-3058 (1980), CA94(12):92726h, Eng. transl., Russ. J. Inorg. Chem., 25, 1676-1679 (1980), force constant, bond length

81ARM/HAL Armentrout, P.B., Halle, L.F., Beauchamp, J.L., "Periodic trends in transition metal-hydrogen, metal-carbon, and metal-oxygen bond dissociation energies. Correlation with reactivity and electronic structure", J. Am. Chem. Soc., 103, 6501-6502 (1981), CA95(18):156742r, ionization potential, dissociation energy

81BAG/BJO Bagus, P.S., Bjoerkman, C., "Electronic structure of transition metal hydrides: nickel hydride (NiH) and palladium hydride (PdH)", Phys. Rev. A, 23(2), 461-472 (1981), CA94(10):71802q, electronic energy levels

81DAS Das, G., "A pseudopotential study of the iron-series transition metal hydrides", J. Chem. Phys., 74(10), 5766-5774 (1981), CA95(2):13166v, dissociation energy

81KHA/KRA Kharitonov, Yu. Ya., Kravtsova, G. V., "Thermodynamic functions of diatomic hydrides of Group VIII metals", Zh. Neorg. Khim., 26(5), 1198-1201 (1981), CA95(4):31394x, Eng. transl., Russ. J. Inorg. Chem., 26, 645-647 (1981), thermodynamic properties

81NIC Nicholls, R. W., "Franck-Condon factor formulas for astrophysical and other molecules", Astrophys. J., Suppl. Ser., 47(3), 279-290 (1981), CA96(8):60604s, Franck-Condon factor

82MET/KUE Methfessel, M., Kuebler, J., "Bond analysis of heats of formation: application to some Group VIII and IB hydrides", J. Phys. F, 12(1), 141-161 (1982), CA96(18):150087e, enthalpy of formation

82SCU/LOE Scullman, R., Loefgren, S., Kadavathu, S. A., "The spectrum of nickel hydride (NiH). Some new transitions", Phys. Scr., 25(2), 295-301 (1982), CA96(20):171521g, electronic energy level

82WAL/BAU Walch, S.P., Bauschlicher, C.W., Jr., "On incorporation of atomic correlation in transition metal molecular calculations: nickel monohydride", Chem. Phys. Lett., 86(1), 66-70 (1982), CA96(18):149486c, dissociation energy

83CAR/SAL Carlin, T.J., Sallans, L., Cassady, C.J., Jacobson, D.B., Freiser, B.S., "Gas-phase reactions of Group VIII metal hydride ions (FeD^+, CoD^+, and NiD^+) with hydrocarbons", J. Am. Chem. Soc., 105(20), 6320-6321 (1983), CA99(17):140141r, ionization potential

83RAJ/RAT Rajulu, A. V., Ratnam, S. R., Reddy, R. R., "Electronegativities in the calculation of diatomic molecular parameters (hydrides of some transition elements)", J. Quant. Spectrosc. Radiat. Transfer, 29(1), 85-88 (1983), CA98(8):62295g, electron affinity

83WAL/BAU Walch, S.P., Bauschlicher, C.W., Jr., "CASSCF/CI calculations for first row transition metal hydrides: the TiH $^4\Phi$, VH $^5\Delta$, CrH $^6\Sigma^+$, MnH $^7\Sigma^+$, FeH $^{4,6}\Delta$, and NiH $^2\Delta$ states", J. Chem. Phys., 78(7), 4597-4605 (1983), CA98(20):167166u, electronic energy level, hydride

84MAN/HAL Mandich, M. L., Halle, L. F., Beauchamp, J. L., "Determination of the metal-hydrogen and metal-methyl bond dissociation energies of the second-row, Group 8 transition metal cations", J. Am. Chem. Soc., 106(16), 4403-4411 (1984), CA101(9):72937n, dissociation energy

84RUE/BLY Ruette, F., Blyholder, G., Head, J., "Bonding and potential energy curves for nickel hydrides (NiH and NiH2)", J. Chem. Phys., 80(5), 2042-2048 (1984), CA100(20):162051c, potential energy curve

84SAU/TAT Sauval, A. J., Tatum, J. B., "A set of partition functions and equilibrium constants for 300 diatomic molecules of astrophysical interest", Astrophys. J., Suppl. Ser., 56(2), 193-209 (1984), CA101(22):200866c, thermodynamic properties

84TSO/KIN Tsong, T. T., Kinkus, T. J., "Energy distributions of pulsed-laser field-desorbed gaseous ions and field-evaporated metal ions: A direct time-of-flight measurement", Phys. Rev. B: Condens. Matter, 29(2), 529-542 (1984), CA100(12):91849f, formation

85BOR/TYU Borodyuk, N. R., Tyulin, V. I., "Calculation of lower limit for the equilibrium internuclear distances in excited electronic states of diatomic molecules", Vestn. Mosk. Univ., Ser. 2: Khim., 26(6), 546-551 (1985), CA104(16):138351n, bond length

85GRA/RIC Gray, J.A., Rice, S.F., Field, R.W., "The electric dipole moment of nickel hydride (NiH) $^2\Delta_{5/2}$ and $B^2\Delta_{5/2}$", J. Chem. Phys., 82(10), 4717-4718 (1985), CA103(2):15406f, electronic energy level, dipole moment

85WAL/BAU Walch, S.P., Bauschlicher, C.W., Jr., Langhoff, S.R., "Calculated electric dipole moment of nickel hydride $(NiH)^2\Delta$", J. Chem. Phys., 83(10), 5351-5352 (1985), CA103(26):225591p, dipole moment, electronic energy level

86CHI/LAN Chiong, D.P., Langhoff, S.R., Bauschlicher, C.W., Jr., Walch, S.P., Partridge, H., "Theoretical dipole moments for the first-row transition metal hydrides", J. Chem. Phys., 85(5), 2850-2860 (1986), CA105(18):163141x, dipole moment

86CHO/LAN Chong, D.P., Langhoff, S.R., "A modified coupled pair functional approach", J. Chem. Phys., 84(10), 5606-5610 (1986), CA105(4):30217e, dissociation energy, bond length

86ELK/ARM Elkind, J. L., Armentrout, P. B., "Transition-metal hydride bond energies: first and second row", Inorg. Chem., 25(8), 1078-1080 (1986), CA104(20):177178f, ionization potential

86GRA/FIE Gray, J. A., Field, R. W., "The Zeeman effect as an aid to electronic assignment: the nickel hydride (NiH) $A^2\Delta_{5/2}$ state", J. Chem. Phys., 84(2), 1041-1042 (1986), CA104(12):98601k, electronic energy level

86KOL/GAG Kolbanovskii, Yu. A., Gagarin, S. G., "Orbital resonance in gaseous reactions between metal monohydride ions and methane", Izv. Akad. Nauk SSSR, Ser. Khim., (6), 1291-1294 (1986), CA105(14):121181e, ionization potential

86ROH/HAY Rohlfing, C.M., Hay, P.J., Martin, R.L., "An effective core potential investigation of Ni, Pd, and Pt and their monohydrides", J. Chem. Phys., 85, 1447-1455 (1986), CA105(12):102957w, electronic energy levels

86SCH/GOD Schilling, J. B., Goddard, W.A., III, Beauchamp, J. L., "Theoretical studies of transition-metal hydrides. 1. Bond energies for MH^+ with M = Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and Zn", J. Am. Chem. Soc., 108(4), 582-584 (1986), CA104(12):95921d, dissociation energy

86SZP/WAL Szpunar, B., Wallace, W. E., Strange, P., "Spin-polarized electronic structure calculations for nickel and nickel hydride (NiH)", J. Less-Common Met., 123, 37-45 (1986), CA106(2):9541s, enthalpy of formation

87ADA/LOE Adakkai Kadavathu, S., Loefgren, S., Scullman, R., "Rotational analysis of some new transitions in nickel deuteride (NiD). A comparison between nickel hydride (NiH) and nickel deuteride (NiD)", Phys. Scr., 35(3), 277-285 (1987), CA106(22):185285v, rotational analysis, electronic energy levels

87MIL/FEI Miller, A.E.S., Feigerle, C.S., Lineberger, W.C., "Laser photoelectron spectroscopy of CrH^-, CoH^-, and NiH^-: periodic trends in the electronic structure of the transition-metal hydrides", J. Chem. Phys., 87(3), 1549-1556 (1987), electron affinity, electronic energy levels, vibrational analysis

JANAF THERMOCHEMICAL TABLES - NICKEL BIBLIOGRAPHIES
NICKEL IODIDE (NiI, NiI^+, NiI^-)

61BUL/PHI Bulewicz, E.M., Phillips, L.F., Sugden, T.M., "Determination of dissociation constants and heats of formation of molecules by flame photometry. VIII. Stabilities of the gaseous diatomic halides of certain metals", Trans. Faraday Soc., 57, 921-931 (1961), CA56:73f, dissociation energy

74BAR/CER Bartovska, L., Cerny, C., Bartovsky, T., "The study of systems cobalt-iodine and nickel-iodine at higher temperatures", Coll. Czech. Chem. Commun., 39, 917-923 (1974), dissociation energy

83KEH/AHL Kehlenbeck, G., Ahlert, J., Wolf, F., Ziegeler, L., Smend, F., Schumacher, M., "Electronic rearrangement on molecules accompanying β-decay investigated by nuclear resonance fluorescence", Z. Physik A, 311(4), 253-257 (1983), CA98(26):223345r, dissociation energy

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Cynthia R. Jackson and Malcolm W. Chase

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A bibliographic collection is provided on data which are necessary for the calculation of the thermochemical properties of the gaseous metal halides, hydrides (deuterides) and their positive and negative ions (MX, MX^+ and MX^-), where M = Co, Fe, and Ni and X = Br, Cl, F, H(D), and I. This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties of these substances for the JANAF Thermochemical Tables.

The collection contains references which have been published through the end of 1986 with some 1987 references. Fifteen bibliographies are given, one for each species. In all bibliographies, the references are listed chronologically; alphabetically by first author within each year. The names of the species are given according to the Chemical Abstracts system of nomenclature (as of the Tenth Collective Index) when possible. The Chemical Abstracts Registry Numbers, if assigned, are also given for each of the species. A brief summary of the type of available information is given.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

bibliography; electron affinity; electronic energy levels; equilibrium data; formation properties; ionization potential; molecular structure; review articles; thermochemistry; thermodynamic properties; transition metal halides and hydrides; vibrational frequencies

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